Use of a continuous integration and deployment software to automate nuclear data V&V

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BROOKHAVEN NATIONAL LABORATORY

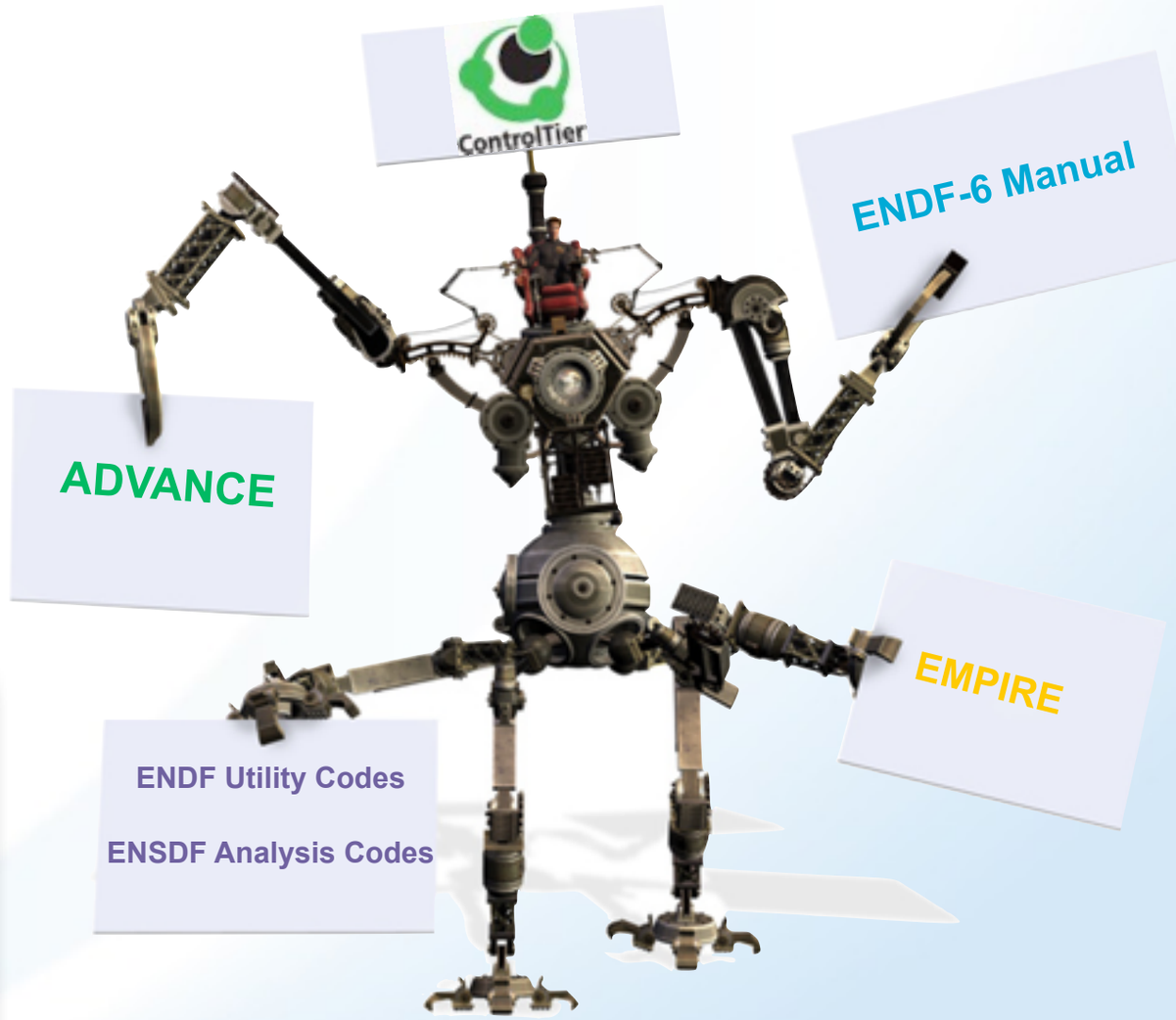
a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

2/3 of BNL's NCSP Nuclear Data tasks are now fully automated

- ☑ Perform data verification of new NCSP evaluations and store them on GForge server (Q1, Q2, Q3, Q4)
- ☑ Perform QA of new NCSP covariance data (Q2, Q4)
- ☐ Update Atlas of Neutron Resonances (Q4)

Our scheme is so useful, NNDC seeking to automate many other tasks with same system



Benefits of automation are clear

- No waiting for assistance from processing code experts
- Extensive testing with minimum effort
  - Number of new commits verified
    - 1 deuteron-incident evaluation
    - 5 decay evaluations
    - 111 neutron-incident evaluations
- High-quality evaluations due to extensive and frequent testing
- Evaluation QA anywhere, anytime through Web at http://www.nndc.bnl.gov/endf/b7.dev/qa/
- Timely feedback on every change enables easier ID and correction of deficiencies

Expected Result

- Expedited submission of evaluations for CSEWG review
- Faster release of new evaluated data libraries

Why did we do it?

What's the Problem?

- Data verification and data validation (V&V) is tedious, so evaluators usually "forget"
- Not all evaluators know how to run the commonly used V&V codes
- Evaluators may have different versions (read: different bugs) of the same V&V code thereby producing different results

What's the solution?

- A highly automated, modular V&V system publicly accessible to evaluators

Automated Data Verification and Assurance for Nuclear Calculations Enhancement (ADVANCE)

Outline

- Motivation
- Benefits of ADVANCE
- The ADVANCE ND/QA System
  - ADVANCE System Architecture
  - ADVANCE Process Flow
  - Future Directions

ADVANCE: The ENDF Continuous Integration System

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ENDF B-VII.dev

ENDF/B Development

The development version of the Evaluated Nuclear Data File (ENDF/B)

Latest Updates

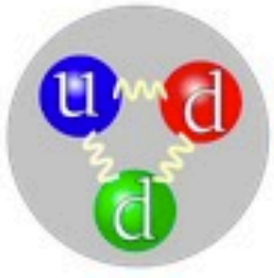
sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 16:57:39.661872

sublib_html: neutrons
Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

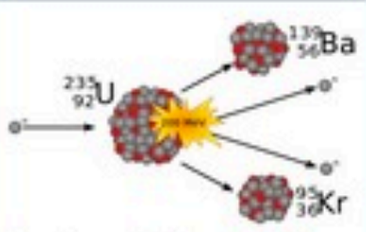
sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 15:41:29.746913

Neutrons | Decay | Charged particles | Photonuclear | Atomic

Neutrons sublibraries



Neutrons Sublibrary



Neutron-Induced Fission Yields Sublibrary

Standards Sublibrary

Thermal Neutron Scattering Sublibrary

Neutrons Sublibrary

ENDF/B Development Library

- General Information:
  - ENDF sublib designator: 10
- Revision Number: 611M
- Last Modified Revision: 532:611M
- Build Status:
  - Build status: ERROR
  - Build time: 2013-04-30 16:52:01.394282
  - Listfile: neutrons.list
  - Release Notes: neutrons-releaseNotes.pdf
- GForge Links:
  - Browse SVN
  - Browse sublibrary tracker

Latest Updates

sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 16:57:39.661872

evaluation_summary: n-098_Cf_251.endf
Code evaluation_summary completed run on n-098_Cf_251.endf. The result was a SUCCESS
2013-04-30 16:52:41.503573

sublib_html: neutrons
Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

Periodic Table | Material List

1 H								X								2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe

- Build status: ERROR
- Build time: 2013-04-30 16:52:01.394282
- Listfile: neutrons.list
- Release Notes: neutrons-releaseNotes.pdf

Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

- GForge Links:
  - Browse SVN

Pu

Status	Material	MAT #	Revision #	# Tests	# Failures	# Errors	Lab.	Date	Authors
	236Pu	9428	603	756	0	44	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, et al.
	237Pu	9431	603	1398	0	136	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, et al.
	238Pu	9434	597	1004	0	180	LANL	SEP10	YOUNG, TALOU, KAWANO, KAHLER, CHADWIC
	239Pu	9437	591	1508	0	68	LANL	SEP06	Young, Chadwick, MacFarlane, Derrien
	240Pu	9440	532	1298	0	216	LANL	SEP09	YOUNG, TALOU, CHADWICK, KAHLER, KAWAN
	241Pu	9443	532	924	0	10	ORNL	OCT03	L.Weston, R.Wright, H.Derrien , et al.
	242Pu	9446	603	1268	0	108	BNL+JAEA	AUG11	S.F. MUGHABGHAB , et al. O.Iwamoto, etal
	243Pu	9449	597	536	0	24	SRL,LLNL	JUL76	Benjamin, McCrosson, Howerton
	244Pu	9452	603	846	0	60	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, , et al.
	246Pu	9458	603	850	0	60	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, et al.

* Lanthanides (Lanthanoids)	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
** Actinides (Actinoids)	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

2 He
10 Ne
18 Ar
36 Kr
54 Xe
86 Rn
118 Uuo

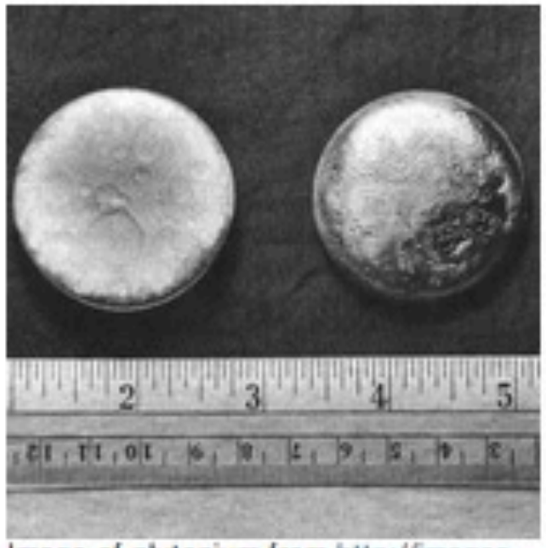


Image of plutonium from http://images-of-elements.com/

^{239}Pu

Neutrons Sublibrary

- General Information:
  - ENDF MAT designator: 9437
  - Evaluated by Young, Chadwick, MacFarlane, Derrien (LANL), SEP06
  - Natural abundance: 0.0 +/- 0.0 %
  - Check out Wikipedia's entry for plutonium
- Revision Number: 611M
- Last Modified Revision: 532:611M
- Build Status:
  - Build status: ERROR (Submit tracker item)
  - Build time: 2013-04-30 06:17:38.108808
- GForge Links:
  - Browse SVN
  - View current revision
  - Download current revision

Latest Updates

evaluation_summary: n-094_Pu_239.endf
Code evaluation_summary completed run on n-094_Pu_239.endf. The result was a SUCCESS
2013-04-30 06:17:39.392055

njoy2012: n-094_Pu_239.endf
Code njoy2012 completed run on n-094_Pu_239.endf. The result was a ERROR
2013-04-30 06:17:36.872836

inter: n-094_Pu_239.endf
Code inter completed run on n-094_Pu_239.endf. The result was a SUCCESS
2013-04-30 06:10:24.995505

Code Results | ENDF Overview | ACE Overview | Integral Quantities | Cross Section Plots

Summary of all tests on this evaluation.

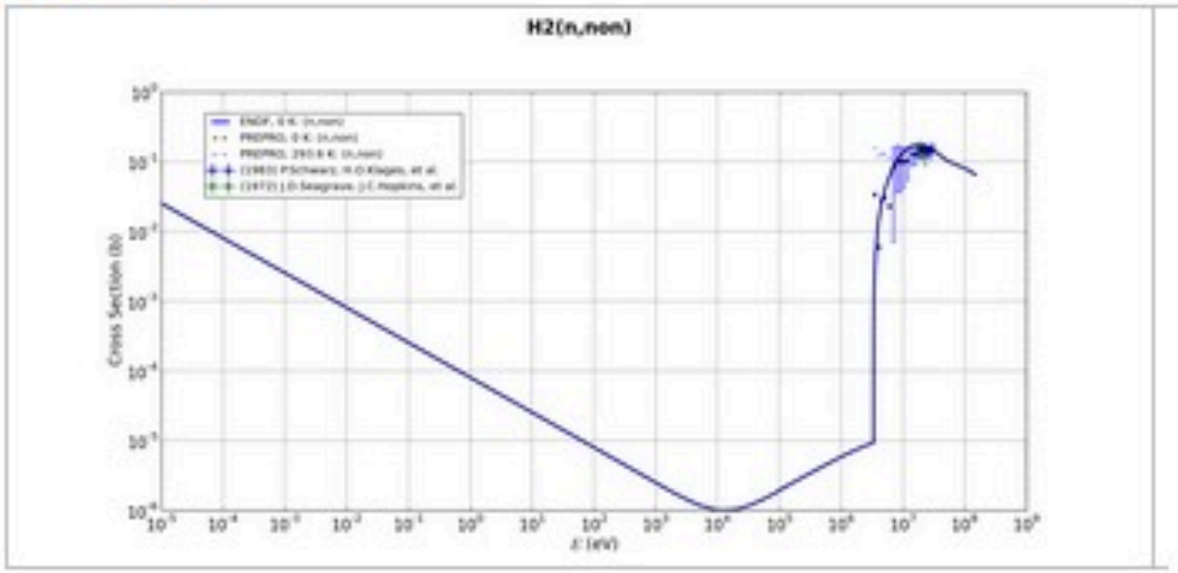
Use checking code button to show/hide errors.

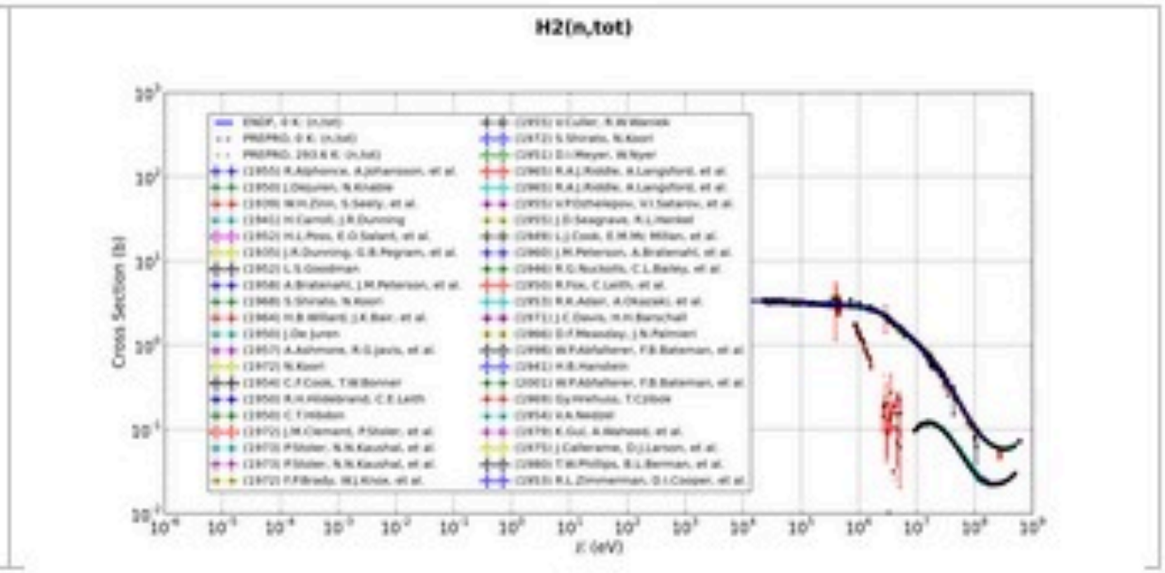
Status	Code	# Tests	# Failures	# Errors	Run time (sec)	Files
✓	STAN	0	0	0	31.533	STN File
✓	STANEF	0	0	0	29.316	

Code Results | ENDF Overview | ACE Overview | Integral Quantities | Cross Section Plots

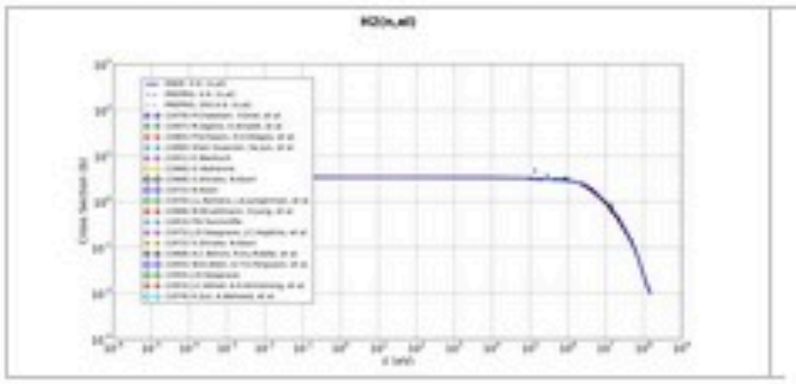
Comparison between cross section data in this ENDF file and data retrieved from EXFOR

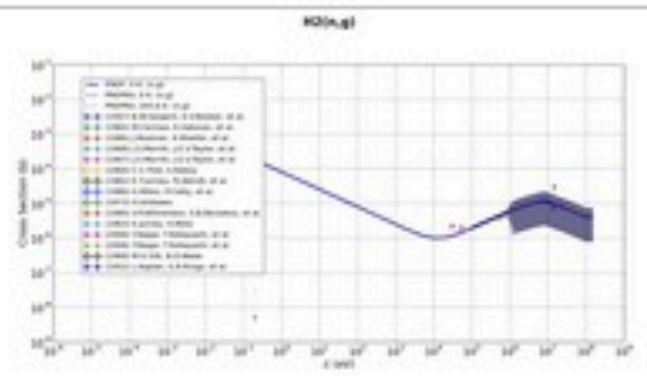
Aggregate channels:

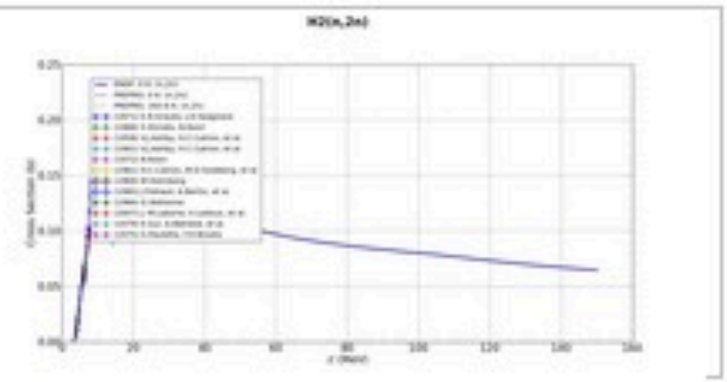




Regular channels:







ADVANCE Version 0.7 (svn rev: 669)

Codes used in ADVANCE version 0.7

- **NNDC checking codes**
  - STAN
  - STANEF
  - CHECKR
  - FIZCON
  - PSYCHE
- **PREPRO**
  - LINEAR
  - RECENT
  - SIGMA1
- **NJOY2012 (upgraded from NJOY99)**
  - grouping, heating, checking
  - ACE file
- **Fudge-4.0 (upgraded from Fudge-2.0)**
  - checking
  - cross section plotting
  - xml/html5 overview
- **Other Codes**
  - INTER: integral quantities
  - ACELST: ACE file overview
  - ENDF2HTM: ENDF overview
  - x4i: EXFOR data for plotting

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ADVANCE System Architecture

Evaluation environment

ENDF Evaluator

ENDF file commits

Verification results

Integration + deployment environment

ENDF File Versioning

GForge Server
(NNDC Ensemble)

SVN check out

Data verification

CI + CD Server

Publish

NNDC Web Server

- GForge Server as the versioning system (Subversion).
- Each commit to ENDF repository triggers data verification
- Results automatically posted on NNDC Web server

The ADVANCE ND/QA System (continued)

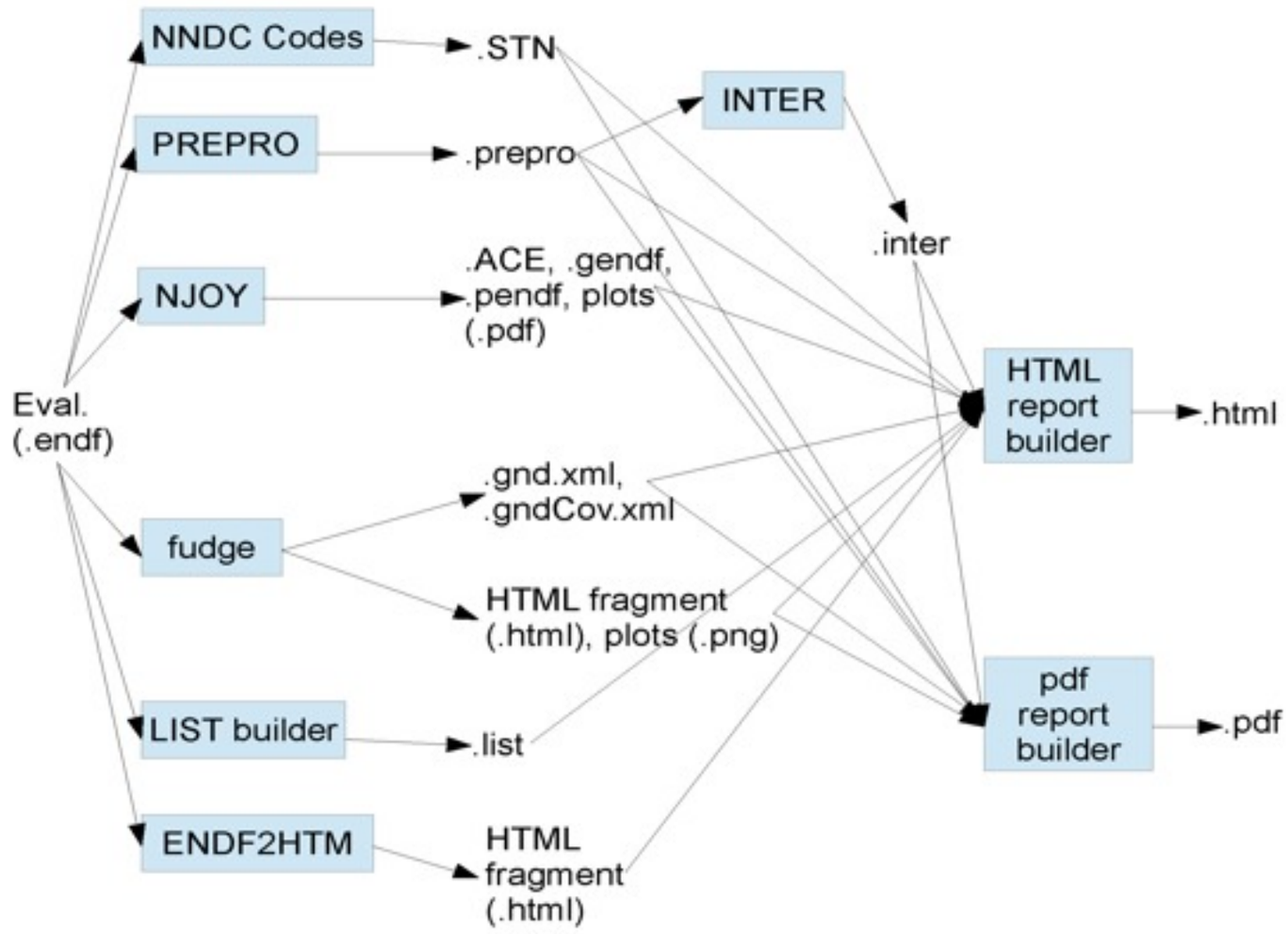
Why ControlTier?

- Robust and reliable
- Cost-free: Good for NNDC's tight budget
- Open-source: Can change system code
- Platform independent: 100% Java
- Most complete platform:
  - Continuous integration + continuous deployment
- Highly scalable: Add servers + clients as needed

ControlTier

ADVANCE Process Flow

Data Verification



Code Dependencies

- A code may depend on output of another code. Thus, a code may not begin processing until the immediate preceding code completes.
- If new commit does not modify input file to a code, then the code and its dependent codes are not executed.

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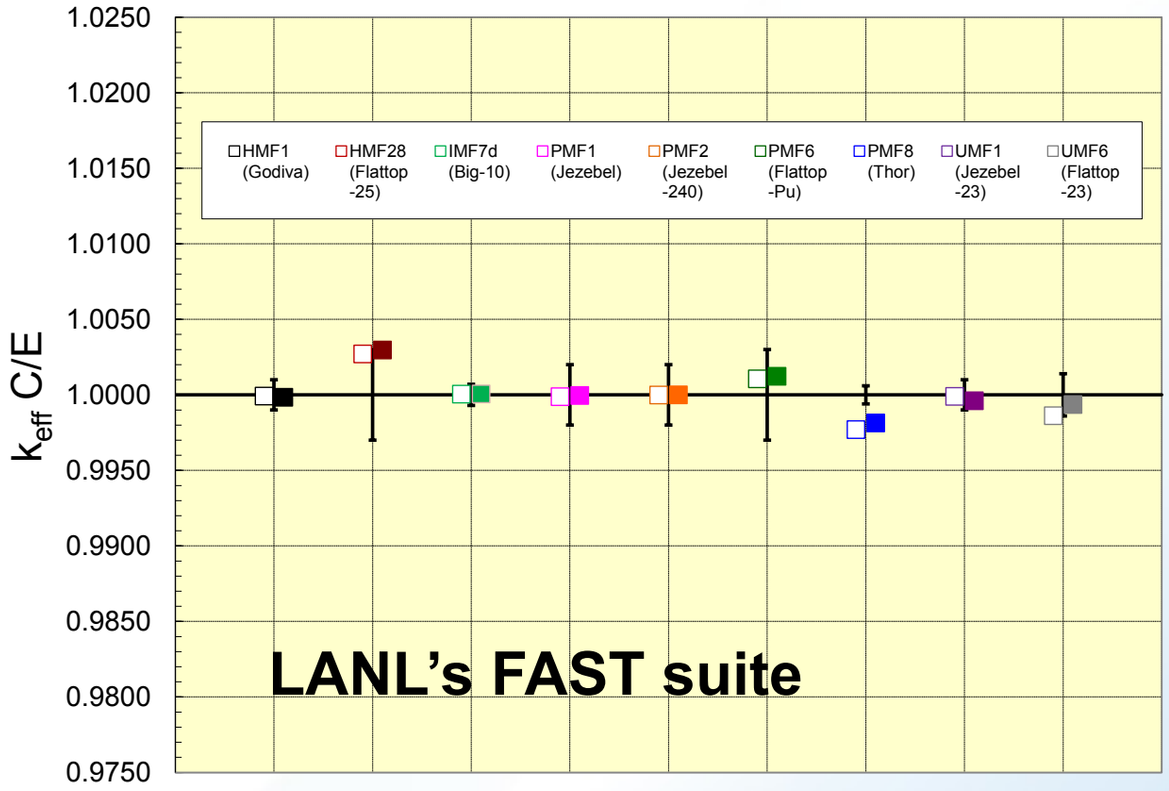
Rest of FY13 plans (in addition to ENDF upkeep)

- **More reports**:
  - Plots of integral quantities (MACS, RI, Cf spectrum ave.)
  - Better energy balance report
  - Covariance QA report
- **Full library tarballs** (ACE, gnd, gendf)
- **More processing codes:**
  - PREPRO/sigma1, sixpack
  - CALENDF
  - Fudge improvements
  - NJOY improvements
- **Database of errors:**
  - [x] processing code error mining
  - regressions
- **Notifications**
  - [x] RSS Feed
  - Emails
- **Help pages**
- **Unit tests/docs**
- **About ADVANCE pages**
- **An ADVANCE paper**
- **Prepare for benchmarking?**

Next logical step: automate simulation of critical assemblies and other benchmarks

- **Criticality benchmarks are already the core of our data testing regimen**
- **Many other tests check things of importance to NCSP**
  - Reaction rates in irradiated foils target individual reactions
  - SINBAD shielding benchmarks can be used to benchmark decay/ activation data



Current testing is human-driven and ad-hoc:

- **We often test outdated libraries (ENDF/B-V??)**
- **We rerun same tests (do we need to run JEZEBEL again?)**
- **We often don't run tests because of lack of resources: models, codes computing and/or manpower**

Automated benchmarking is one of NCSP's 5 year goals

Opportunities

- ***cnp_test_suite release***
- **Transport code and test suite donations**
  - ***COG release***
  - COG suite release
  - ***MCNP6 release***
  - Mosteller suite of 119 tests
  - BNL 1D Sn tests
- **NNDC cluster upgrade:** cluster size to double to 184 Intel Xeon nodes
- **ADVANCE master node upgrade**

Challenges

- **NNDC webserver upgrade:** may force adoption of web content management system instead of static web pages for reports
- **ControlTier project ended:** in long term must switch control system to either RunDeck or BuildBot or similar

We would like to develop a meaningful requirements documentation

Gathering requirements for next major release of ADVANCE

- **More processing codes**: AMPX
- **Local (NNDC) benchmarking**
  - Using MCNP6, ANISN, TWOTRAN and COG
- **Hooks for remote benchmarking**
  - LLNL CNP group collaboration
- **Try/accept functionality** (try an evaluation before committing to GForge)
- **Better notifications**
- **CMS for better report management**
- **Comments subsystem**
- **Better functionality for CI/CD for non-data projects** (e.g. EMPIRE)
- **Open source release**

What else?

Acknowledgments

Many thanks to C. Mattoon (LLNL), B. Beck (LLNL), N. Summers (LLNL) and M.-A. Descalle (LLNL) for the advice and valuable assistance they provided especially at the early stage of the ADVANCE project and for providing us with LLNL's cnp_test_suite package.

D. Heinrichs and C. Lee for preparing COG for general release.